

be a 3-quasi-particle intruder state. In the investigations carried out by the present authors⁵ the 321 keV state was observed to be more of a phonon addition type to the 145 keV ($h_{11/2}$) state. If the 642 keV state has a character of $7/2^+$, it may be interpreted as a $g_{7/2}$ state or a $g_{7/2}$ particle part admixed to the phonon addition to other particle states in the major shell ($d_{5/2}$, $d_{3/2}$ and $s_{1/2}$). It is rather difficult to explain under these conditions the predominant E1 nature of the 321 keV transition.

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succeeded in tracing out the P and R equally intense branches due to these isotopes in (0, 1) and (2, 0) bands. Respective combination differences between P and R branches of $^{63}\text{Cu}^{81}\text{Br}$ for (0, 1) and (2, 0) were compared with the respective bands of C-X system analysed by Rao and Rao.² The rotational isotopic shifts in the P and R branch lines due to $^{63}\text{Cu}^{81}\text{Br}$ have been found to be in good agreement with the calculated shifts. The rotational constants are summarized in Table I.

TABLE I

Molecular constants of D-X system of CuBr

(0, 1)	(2, 0)
$^{79}\nu_0 = 25211.20 \text{ cm}^{-1}$	$^{79}\nu_0 = 26077.50 \text{ cm}^{-1}$
$^{81}\nu_0 = 25209.30 \text{ cm}^{-1}$	$^{81}\nu_0 = 26074.30 \text{ cm}^{-1}$
$^{79}B_0' = 0.0926 \text{ cm}^{-1}$	$^{79}B_2' = 0.0907 \text{ cm}^{-1}$
$^{79}B_1'' = 0.1005 \text{ cm}^{-1}$	$^{79}B_0'' = 0.1004 \text{ cm}^{-1}$
$^{81}B_0' = 0.0917 \text{ cm}^{-1}$	$^{81}B_2' = 0.0895 \text{ cm}^{-1}$
$^{81}B_1'' = 0.0995 \text{ cm}^{-1}$	$^{81}B_0'' = 0.0993 \text{ cm}^{-1}$

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ROTATIONAL ANALYSIS OF D-X BAND SYSTEM OF CuBr MOLECULE

Four band systems are known for the CuBr molecule, namely, A system (4600-5100 Å), B system (4200-4600 Å), C system (3900-4000 Å) and D system (3700-4000 Å). The A, B, C systems have been analysed by Ritschel¹ and Rao and Rao.² The D system was obtained in emission recently by Rao and Rao.³ These four band systems have a common lower $X^1\Sigma$ state as the ground state of the molecule.

In the present study, the bands of D system of CuBr molecule have been photographed in the second order of 10.6 meter concave grating spectrograph having the dispersion 0.33 Å/mm. The rotational analyses of (2, 0) and (0, 1) bands have been carried out.

The transition of D system was predicted as $^1\Sigma^- \rightarrow ^1\Sigma^+$ by Rao and Rao.³ Due to two equally abundant isotopes, i.e., $^{63}\text{Cu}^{79}\text{Br}$ and $^{63}\text{Cu}^{81}\text{Br}$ (7:7) the rotational structure of the bands presents a complex look. However, we have

DEBYE PARAMETER AND VIBRATION AMPLITUDE OF SODIUM

ABSTRACT

Accurate Bragg intensity data at room temperature were collected from three single crystals of metallic sodium grown from melt, using $\text{CuK}\alpha$ radiation in the equi-inclination Weissenberg setting. The integrated intensities were measured on a microdensitometer and corrected for secondary extinction. Structure factor-least squares refinement of the thermal parameter, with correction for thermal diffuse scattering, gave the final B value at 300°K as $B = 7.61 \pm 0.08 \text{ \AA}^2$. The r.m.s. amplitude of thermal vibrations, $(u^2)^{1/2}$, and the Debye characteristic temperature, θ , at 300°K are 0.51 Å, and 140.1°K, respectively.

RECENTLY, the temperature dependence of Debye-Waller factor of Na has been investigated theoretically using the Kretz model, by Singh and Sharma¹. The only experimental work has been the very early X-ray study of Dawton². We have now determined the Debye-Waller factor of metallic sodium, at room temperature from accurate X-ray inten-

sity data from 3 single crystals, grown from melt (along [111] direction), in quartz and Lindemann capillaries. Slowly cooled crystals gave much lower intensities for low angle reflections than fast cooled ones, indicating that the latter were better suited for X-ray diffraction work.

Accurate Bragg intensities of 12 independent reflections, from these 3 samples were collected on multiple films, using $\text{CuK}\alpha$ radiation, in the equi-inclination Weissenberg setting. The integrated intensities were measured on a microdensitometer. The intensity data were corrected for Lorentz-polarisation factor, spot shape, and absorption. Cromer and Waber³ form factors, f_{Na} , corrected for anomalous dispersion were used. Figure 1 shows the presence of extinction effects on the low angle

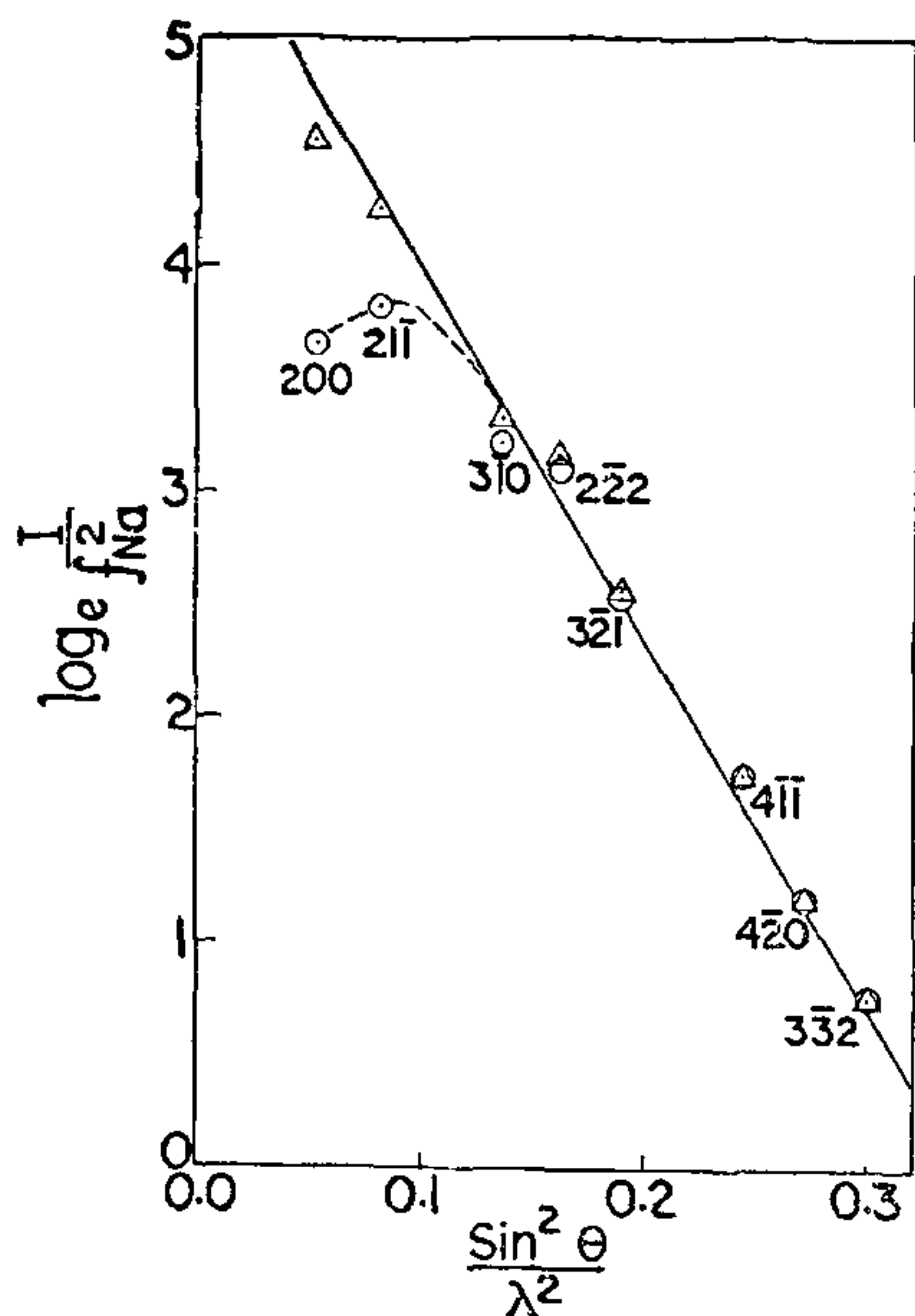


FIG. 1. \odot Intensities not corrected for extinction.
 \triangle Intensities corrected for secondary extinction.

reflections. The final B value was obtained by structure factor least squares refinement using secondary extinction corrected intensities, with g factors of 0.0022, 0.0048 and 0.0061, for samples 1, 2 and 3 respectively.

Table I gives the results of the present study. B_{TDS} refers to B value corrected for thermal

diffuse scattering, by Lucas method⁴, the required elastic constants having been taken from Daniels⁵. Also listed in the table is the B value at room temperature as taken from the plot given by Singh and Sharma¹, theoretically calculated on the Krenb's model. This plot gives the values of $(B_r - B_0)$ only. With the reference B_0 taken equal to that calculated from Dawton's intensities given at the lowest temperature (117° K), the B value at room temperature 300° K is equal to 5.1 Å².

TABLE I

Observed, F_o , and calculated, F_c , structure factor data (given for sample 1 only). Debye parameter, B, Debye characteristic temperature, Θ , and r.m.s. amplitude of thermal vibrations, $(\bar{u}^2)^{1/2}$, at room temperature are also given.

<i>h</i>	<i>k</i>	<i>l</i>	No. of measurements	F_o	F_c
2	0	0	4	11.10	11.11
1	1	2	26	8.51	8.36
2	0	2	19	6.40	6.33
3	1	0	24	4.64	4.82
2	2	2	2	3.91	3.69
1	2	3	40	2.88	2.84
4	0	0	4	2.13	2.20
3	0	3	6	1.72	1.70
4	1	1	12	1.61	1.70
4	2	0	5	1.12	1.33
3	3	2	4	0.93	1.04
2	2	4	2	0.81	0.82

R-factor : 2.55% ; $B = 6.94 \text{ \AA}^2$ (E.S.D. in $B = 0.08 \text{ \AA}^2$).

Present value, with TDS correction (averaged over the 3 samples):

$B_{\text{TDS}} = 7.64 \pm 0.08 \text{ \AA}^2$; $\Theta = 140.1^\circ \text{K}$; $(\bar{u}^2)^{1/2} = 0.54 \text{ \AA}$.

Dawton's²: $B = 6.87 \text{ \AA}^2$; $\Theta = 146.0^\circ \text{K}$.

(calculated from his intensity data)

Singh and Sharma¹: $B = 5.1 \text{ \AA}^2$.

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